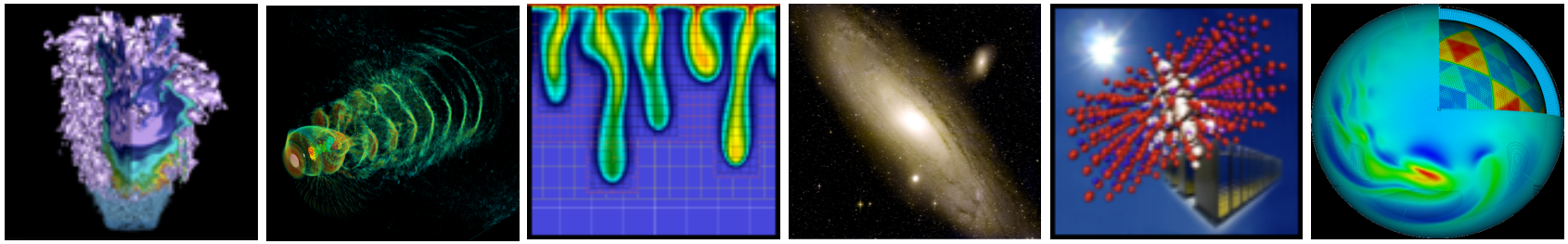

NOVA

NERSC's Online VASP Application

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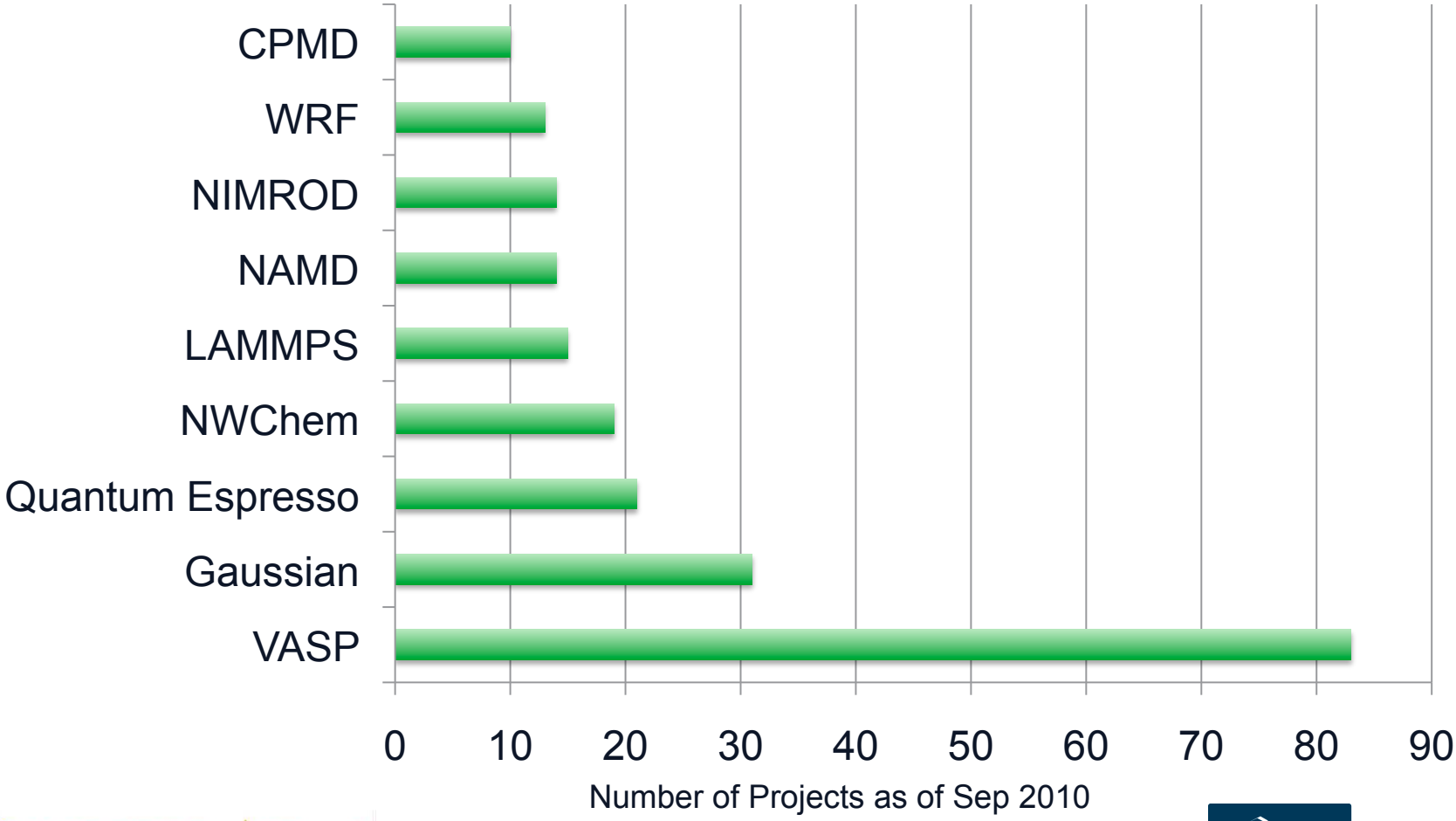
U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC National Energy Research Scientific Computing Center

BERKELEY LAB Lawrence Berkeley National Laboratory

Why VASP?

Codes Used by the Most Projects at NERSC



Why run VASP in a browser?

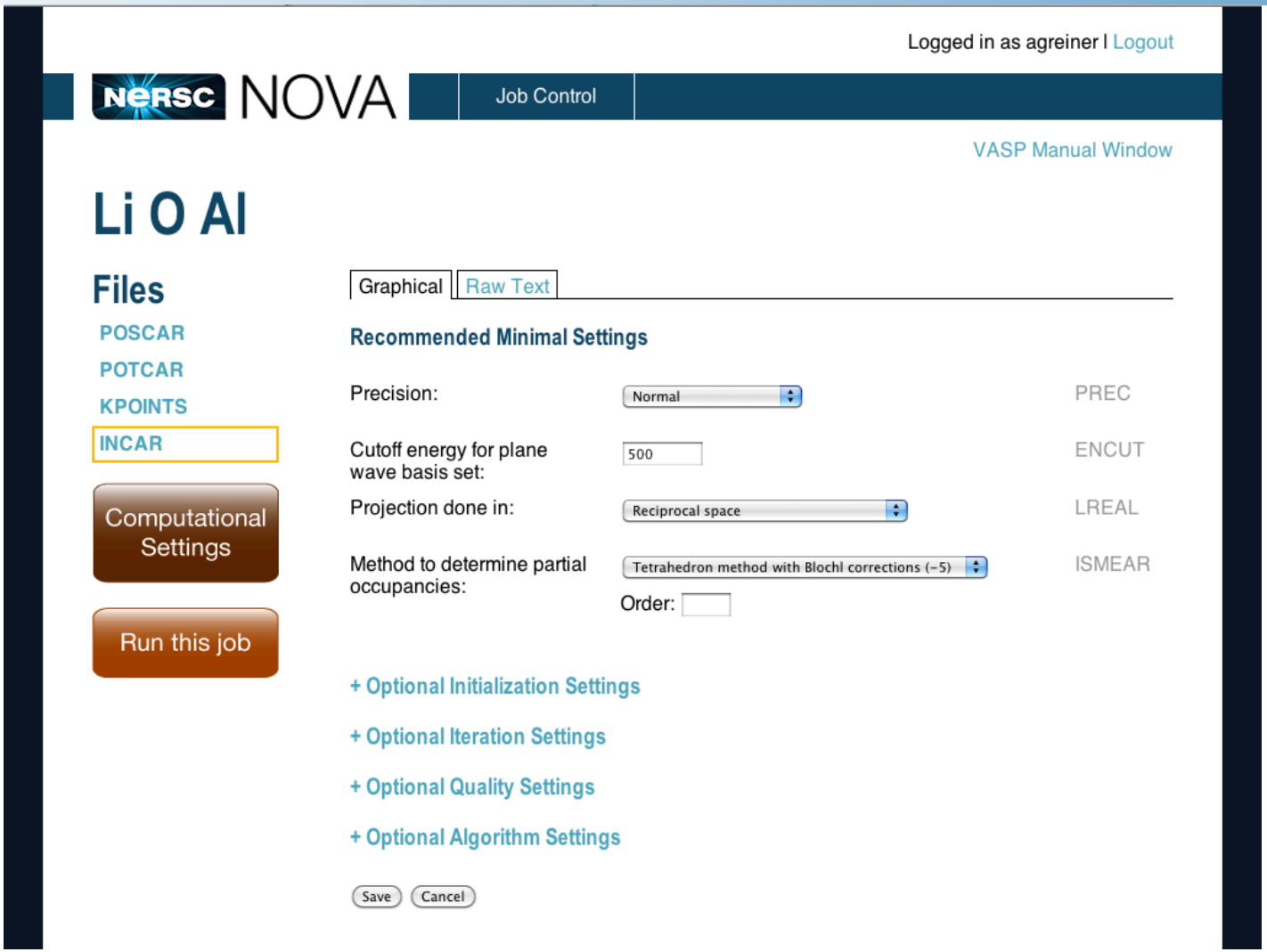
Making interacting with HPC more efficient

- Error checking
- Organizing and retrieving jobs
- Real-time job monitoring
- Integrated analysis tools
- Integration with other online tools
- Meaningful UI controls

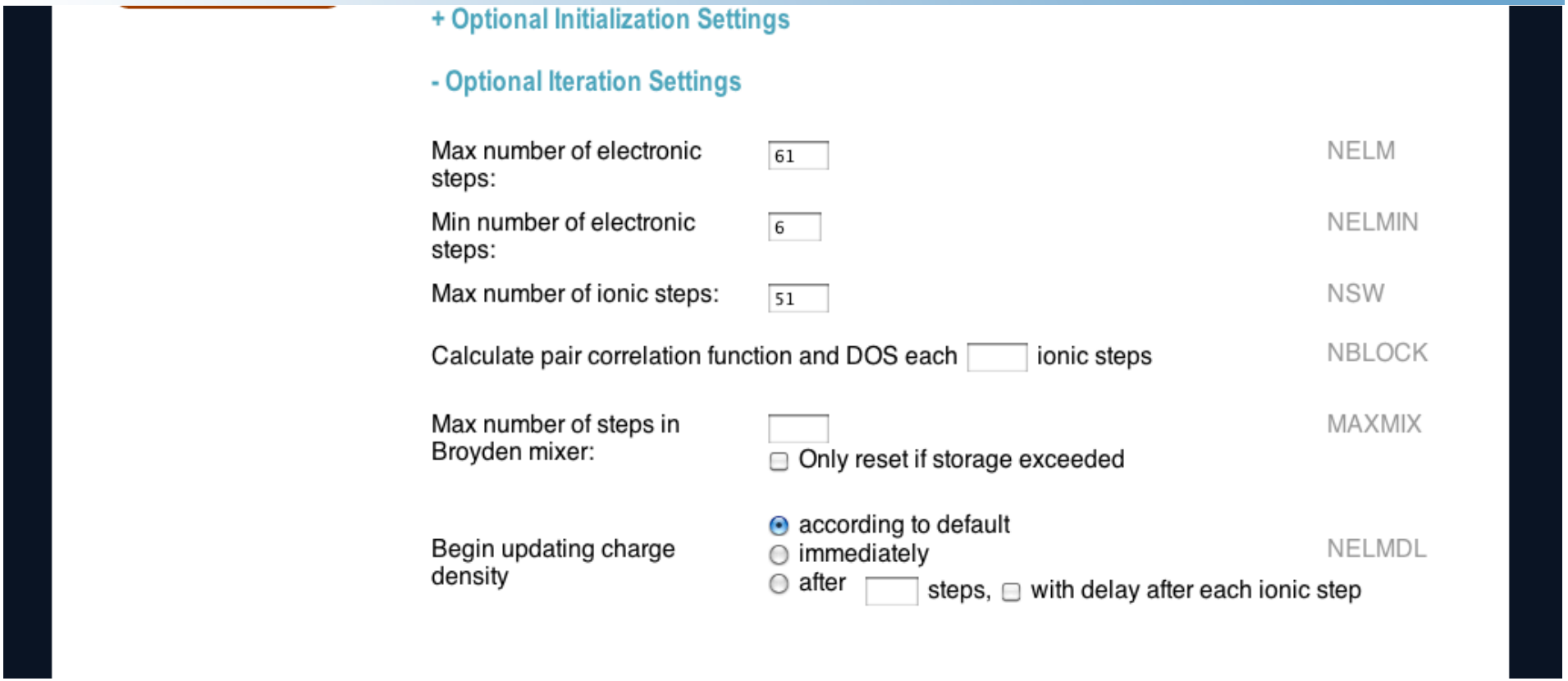
VASP with a modern interface

```
 SYSTEM =  Hg

  NWRITE = 2
  IALGO  = 48 ! uncomment this line to get timings
  NELM = 13
  ENMAX  = 140 eV ; IALGO = -1 ; NELMIN = 3 ; NELMDL = 7
  NGX=31 ; NGY=31 ; NGZ=31 ; NGXF=48 ; NGYF=48 ; NGZF=48
  NBANDS=316
  NSIM  =4

  LREAL  = .TRUE.    real space projections
  BMIX   = 2.5       mixing parameter
  ISYM   = 0         switch of symmetry
  EDIFF  = 1E-4
  LWAVE=.FALSE.
  LCHARG=.FALSE.

Ionic Relaxation
  NSW    =       0    number of steps for IOM
  NBLOCK = 1 ; KBLOCK =  5
  SMASS  =     0.5    Nose mass-parameter (am)
  POTIM  =    5.00    time-step for ion-motion
  TEBEG  =    423     temperature

 PC-function
  APACO  = 10.0      distance for P.C.

 Mass of Ions in am
  POMASS = 200.59000
  ZVAL   =  12.00
```

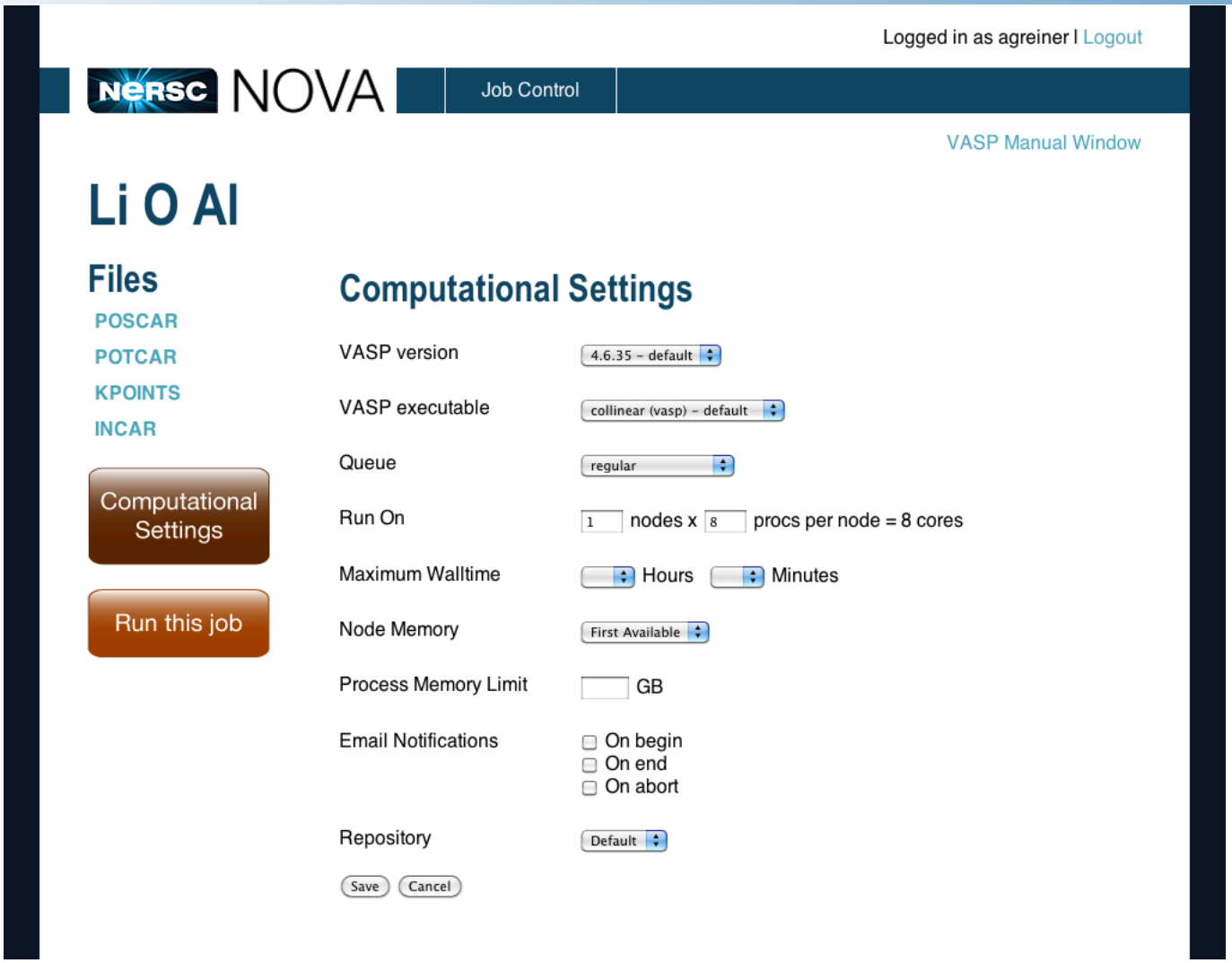
VASP with a modern interface



VASP with a modern interface

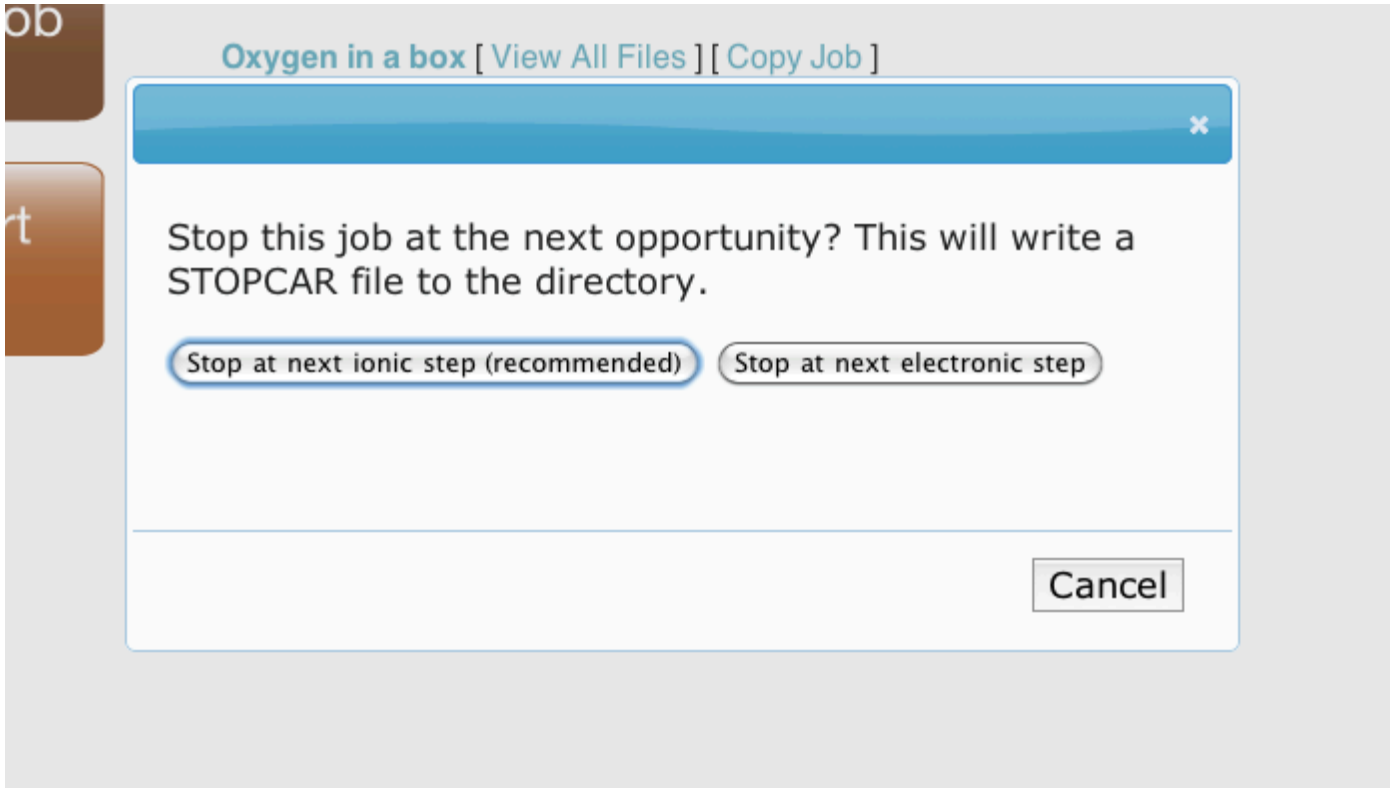


VASP with a modern interface



VASP with a modern interface

Real-Time Monitoring



Real-Time Monitoring

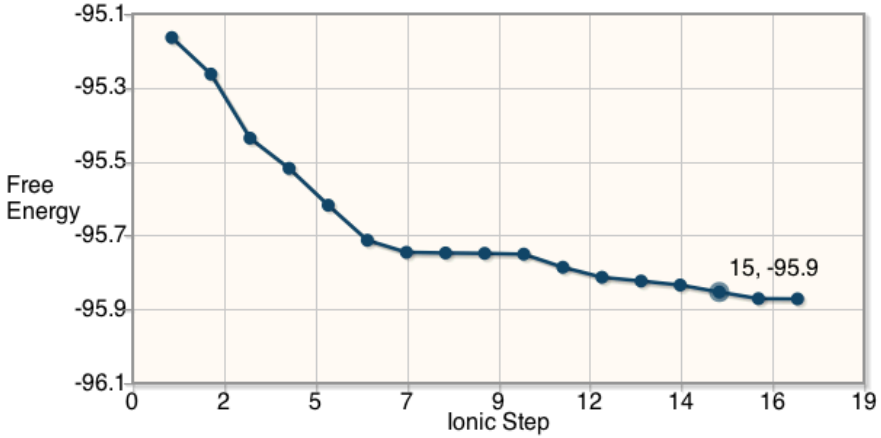
Logged in as agreiner | Logout

NERSC NOVA | Job Control

VASP Manual Window

Li O Al

Convergence



Job Information

System: carver

PBS Job ID: 606410.cvrsvc09-ib

Current State of NOVA

- Django application using the NEWT API
- Early version implements some graphical features
- Checks INCAR keywords and values
- Can set up jobs, copy, submit, monitor, stop, import files from outside NOVA

Future Features

- Real-time convergence monitoring
- POSCAR file generation
- Ensured coherency across input files
- Visualization tools
- Advanced error detection
- File sharing
- Connection to Materials Genome Project

Available April 11

Test version of NOVA

https://portal-auth.nersc.gov/nova

Comments and suggestions to
amgreiner@lbl.gov

National Energy Research Scientific Computing Center